

chain nodes :

11 13 14 16 17

ring nodes :

1 2 3 4 5 6 7 8 9 10

chain bonds :

7-13 16-17

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10

exact/norm bonds :

7-13 16-17

normalized bonds :

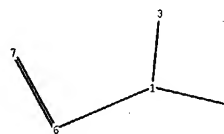
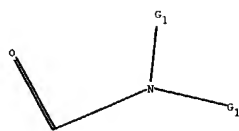
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS



chain nodes :

1 3 4 6 7

chain bonds :

1-4 1-3 1-6 6-7

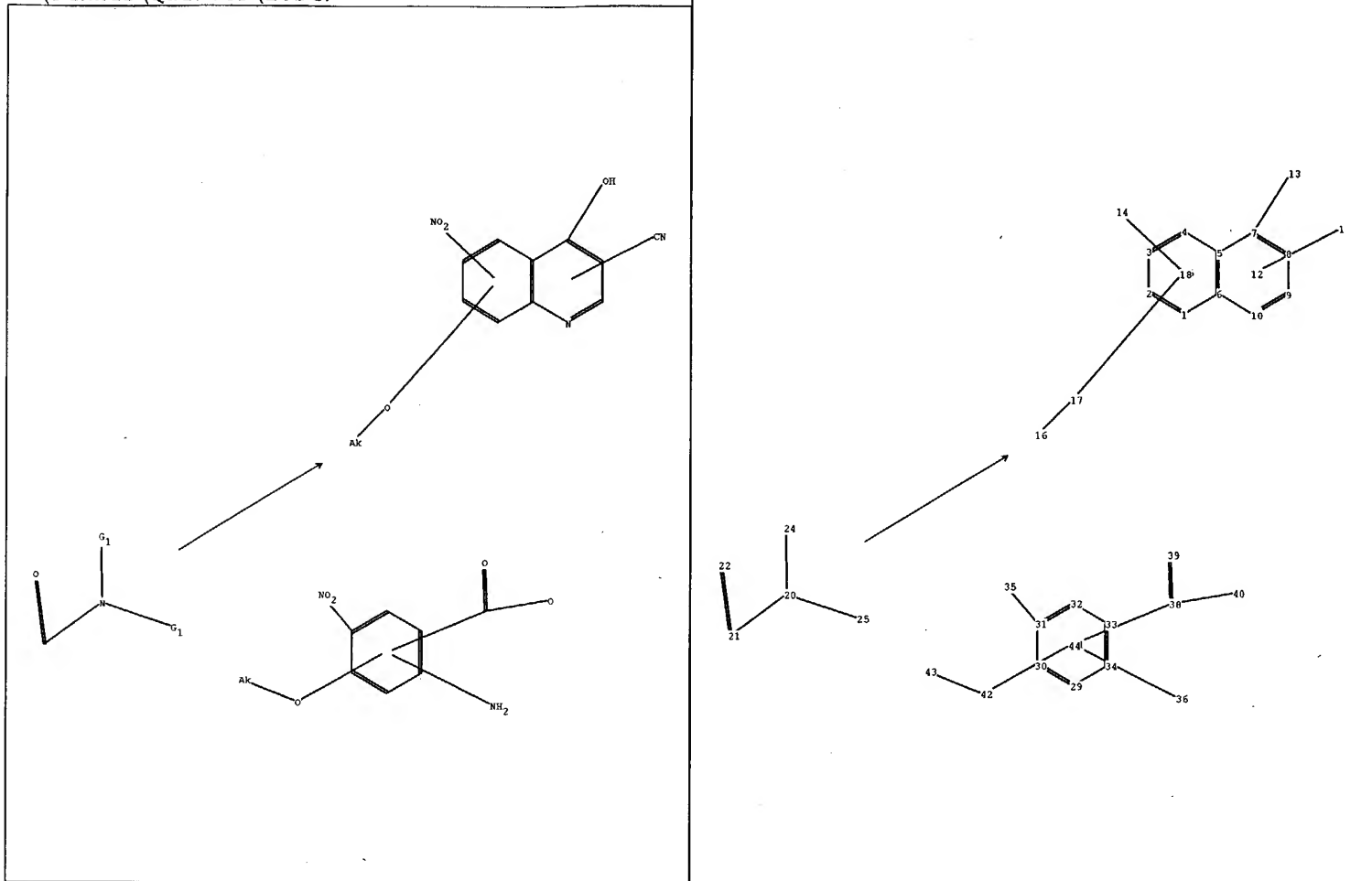
exact/norm bonds :

1-4 1-3 1-6 6-7

G1:CH3,Et

Match level :

1:CLASS 3:CLASS 4:CLASS 6:CLASS 7:CLASS



chain nodes :
 11 13 14 16 17 20 21 22 24 25 35 36 38 39 40 42 43
 ring nodes :
 1 2 3 4 5 6 7 8 9 10 29 30 31 32 33 34
 chain bonds :
 7-13 16-17 20-21 20-25 20-24 21-22 31-35 38-39 38-40 42-43
 ring bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 29-30 29-34 30-31 31-32
 32-33 33-34
 exact/norm bonds :
 7-13 16-17 20-21 20-25 20-24 21-22 38-39 38-40 42-43
 exact bonds :
 31-35
 normalized bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 29-30 29-34 30-31 31-32
 32-33 33-34
 isolated ring systems :
 containing 1 : 29 :

G1:CH3,Et

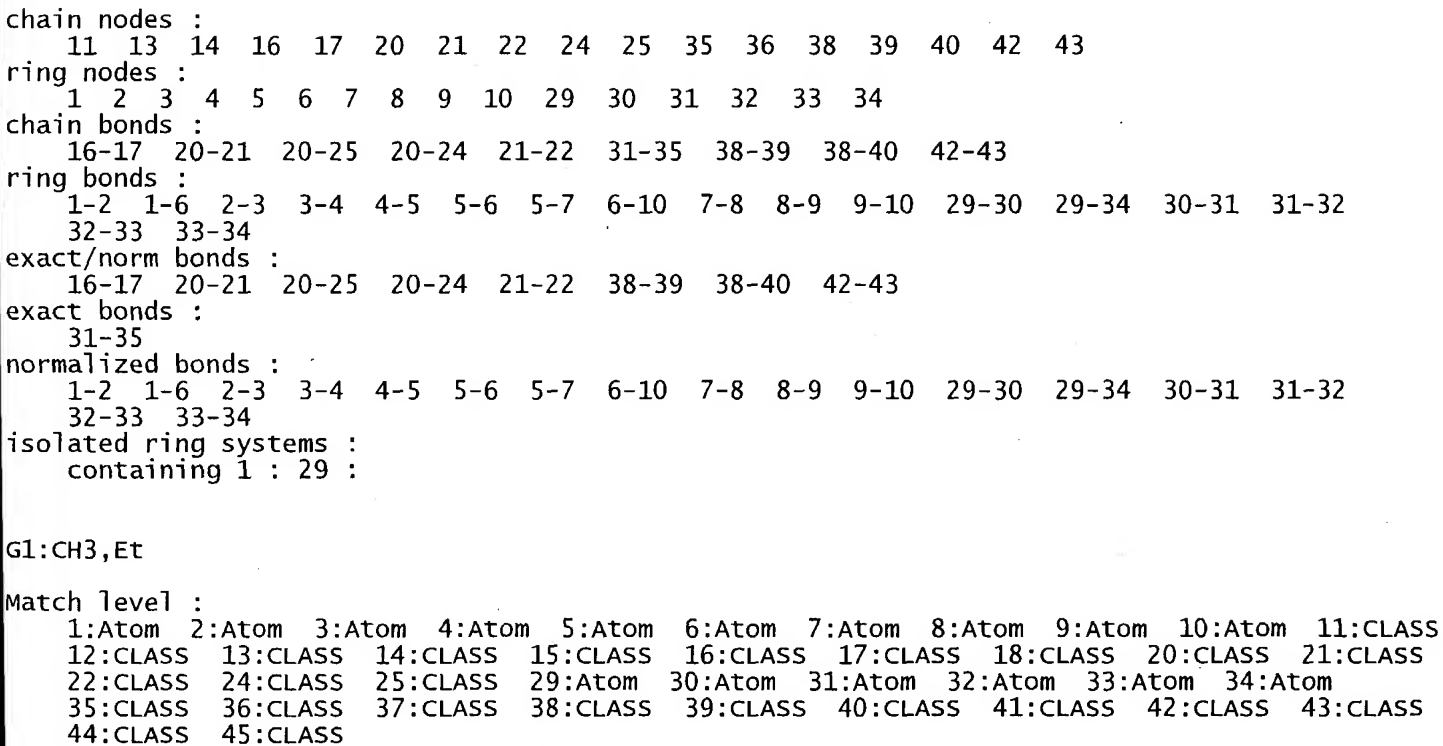
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS
 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS
 22:CLASS 24:CLASS 25:CLASS 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom
 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS
 44:CLASS

fragments assigned reactant role:
 containing 29

fragments assigned product role:
 containing 1

fragments assigned reactant/reagent role:
 containing 20



* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 Jul 12 BEILSTEIN enhanced with new display and select options,
 resulting in a closer connection to BABS
NEWS 4 AUG 02 IFIPAT/IFIUDB/IFICDB reloaded with new search and display
 fields
NEWS 5 AUG 02 Caplus and CA patent records enhanced with European and Japan
 Patent Office Classifications
NEWS 6 AUG 02 The Analysis Edition of STN Express with Discover!
 (Version 7.01 for Windows) now available
NEWS 7 AUG 27 BIOCOMMERCE: Changes and enhancements to content coverage
NEWS 8 AUG 27 BIOTECHABS/BIOTECHDS: Two new display fields added for legal
 status data from INPADOC
NEWS 9 SEP 01 INPADOC: New family current-awareness alert (SDI) available
NEWS 10 SEP 01 New pricing for the Save Answers for SciFinder Wizard within
 STN Express with Discover!
NEWS 11 SEP 01 New display format, HITSTR, available in WPIDS/WPINDEX/WPIX
NEWS 12 SEP 27 STANDARDS will no longer be available on STN
NEWS 13 SEP 27 SWETSCAN will no longer be available on STN

NEWS EXPRESS JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT
 MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
 AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
NEWS HOURS STN Operating Hours Plus Help Desk Availability
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NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 01:37:40 ON 27 OCT 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 01:37:49 ON 27 OCT 2004

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STRUCTURE FILE UPDATES: 25 OCT 2004 HIGHEST RN 769101-30-6
 DICTIONARY FILE UPDATES: 25 OCT 2004 HIGHEST RN 769101-30-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

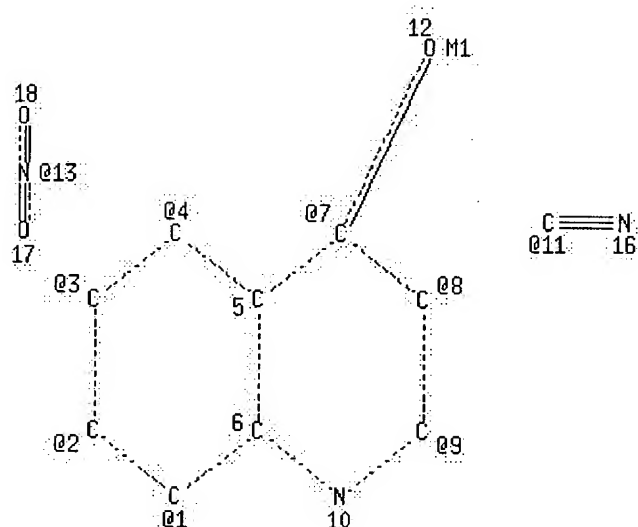
=>

L1 STRUCTURE UPLOADED

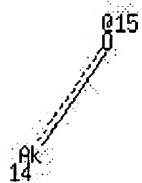
=> d 11

L1 HAS NO ANSWERS

L1 STR



Page 1-A



Page 2-A

VPA 11-7/8/9 S

VPA 13-2/3/4 S

VPA 15-1/2/3 S

NODE ATTRIBUTES:

HCOUNT	IS M1	AT	12
NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS R	AT	7
NSPEC	IS R	AT	8
NSPEC	IS R	AT	9
NSPEC	IS R	AT	10
NSPEC	IS C	AT	11

NSPEC IS C AT 12
 NSPEC IS C AT 13
 NSPEC IS C AT 14
 NSPEC IS C AT 15
 NSPEC IS C AT 16
 NSPEC IS C AT 17
 NSPEC IS C AT 18
 DEFAULT MLEVEL IS ATOM
 MLEVEL IS CLASS AT 11 12 13 14 15 16 17 18
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RSPEC I
 NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

=> s l1
 SAMPLE SEARCH INITIATED 01:40:55 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 16 TO ITERATE

100.0% PROCESSED 16 ITERATIONS 1 ANSWERS
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 80 TO 560
 PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 full
 THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
 FULL SEARCH INITIATED 01:40:59 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 189 TO ITERATE

100.0% PROCESSED 189 ITERATIONS 5 ANSWERS
 SEARCH TIME: 00.00.01

L3 5 SEA SSS FUL L1

=>
 L4 STRUCTURE UPLOADED

=> d l4
 L4 HAS NO ANSWERS
 L4 STR

=> s l4
 SAMPLE SEARCH INITIATED 01:43:05 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 268233 TO ITERATE

0.4% PROCESSED 1000 ITERATIONS 18 ANSWERS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
 BATCH **INCOMPLETE**

PROJECTED ITERATIONS: EXCEEDS 1000000
 PROJECTED ANSWERS: EXCEEDS 92397

L5 18 SEA SSS SAM L4

=> e dimethyl formamide/cn

E1	1	DIMETHYL FLUOROPHOSPHATE/CN
E2	1	DIMETHYL FORMAL/CN
E3	0 -->	DIMETHYL FORMAMIDE/CN
E4	1	DIMETHYL FORMAMIDOMALONATE/CN
E5	1	DIMETHYL FORMYLMALONATE/CN
E6	1	DIMETHYL FORMYLPHOSPHONATE/CN
E7	1	DIMETHYL FORMYLSUCCINATE/CN
E8	1	DIMETHYL FUMARATE/CN
E9	1	DIMETHYL FUMARATE HOMOPOLYMER/CN
E10	1	DIMETHYL FUMARATE POLYMER/CN
E11	1	DIMETHYL FUMARATE RADICAL ION(1-)/CN
E12	1	DIMETHYL FUMARATE-1,1'-(1,2-ETHANEDIYL) BIS(2,2,6,6-TETRAMETHYL-4-PIPERIDINOL) COPOLYMER/CN

=> e dimethyl formamide/cn

E1	1	DIMETHYL FLUOROPHOSPHATE/CN
E2	1	DIMETHYL FORMAL/CN
E3	0 -->	DIMETHYL FORMAMIDE/CN
E4	1	DIMETHYL FORMAMIDOMALONATE/CN
E5	1	DIMETHYL FORMYLMALONATE/CN
E6	1	DIMETHYL FORMYLPHOSPHONATE/CN
E7	1	DIMETHYL FORMYLSUCCINATE/CN
E8	1	DIMETHYL FUMARATE/CN
E9	1	DIMETHYL FUMARATE HOMOPOLYMER/CN
E10	1	DIMETHYL FUMARATE POLYMER/CN
E11	1	DIMETHYL FUMARATE RADICAL ION(1-)/CN
E12	1	DIMETHYL FUMARATE-1,1'-(1,2-ETHANEDIYL) BIS(2,2,6,6-TETRAMETHYL-4-PIPERIDINOL) COPOLYMER/CN

=> e t-butyl cyanoacetate/cn

E1	1	T-BUTYL 6-TRIFLUOROMETHYL-3-(4-PYRIDINYLAMINO) INDOLE-2-CARBOXYLATE/CN
E2	1	T-BUTYL ACRYLATE-DIETHYLENE GLYCOL MONOETHYL ETHER ACRYLATE-BUTYL METHACRYLATE-METHYL METHACRYLATE-METHACRYLIC ACID-DI-T-BUTYL MALEATE COPOLYMER/CN
E3	0 -->	T-BUTYL CYANOACETATE/CN
E4	1	T-BUTYL ETHYL KETONE/CN
E5	1	T-BUTYL HYDROPEROXIDE/CN
E6	1	T-BUTYL IODIDE/CN
E7	1	T-BUTYL METHACRYLATE-1,3-BUTYLENE GLYCOL DIMETHACRYLATE COPOLYMER/CN
E8	1	T-BUTYL METHACRYLATE-DIETHYLENE GLYCOL MONOETHYL ETHER ACRYLATE-2-HYDROXYETHYL METHACRYLATE COPOLYMER/CN
E9	1	T-BUTYL METHACRYLATE-DIETHYLENE GLYCOL MONOETHYL ETHER ACRYLATE-METHACRYLIC ACID COPOLYMER/CN
E10	1	T-BUTYL METHACRYLATE-DIPROPYLENE GLYCOL MONOMETHYL ETHER ACRYLATE-METHACRYLIC ACID COPOLYMER/CN
E11	1	T-BUTYL METHACRYLATE-ETHYLENE GLYCOL MONOPHENYL ETHER METHACRYLATE-METHACRYLIC ACID COPOLYMER/CN
E12	1	T-BUTYL METHACRYLATE-ETHYLENE GLYCOL MONOPHENYL ETHER METHACRYLATE-METHACRYLIC ACID-METHYL METHACRYLATE COPOLYMER/CN

=> d his

(FILE 'HOME' ENTERED AT 01:37:40 ON 27 OCT 2004)

FILE 'REGISTRY' ENTERED AT 01:37:49 ON 27 OCT 2004

```
L1      STRUCTURE UPLOADED
L2      1 S L1
L3      5 S L1 FULL
L4      STRUCTURE UPLOADED
L5      18 S L4
          E DIMETHYL FORMAMIDE/CN
          E DIMETHYL FORMAMIDE/CN
          E T-BUTYL CYANOACETATE/CN
```

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	159.62	159.83

FILE 'HCAPLUS' ENTERED AT 01:44:10 ON 27 OCT 2004

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FILE COVERS 1907 - 27 Oct 2004 VOL 141 ISS 18

FILE LAST UPDATED: 25 Oct 2004 (20041025/ED)

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=> d his

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FILE 'REGISTRY' ENTERED AT 01:37:49 ON 27 OCT 2004

```
L1      STRUCTURE UPLOADED
L2      1 S L1
L3      5 S L1 FULL
L4      STRUCTURE UPLOADED
L5      18 S L4
          E DIMETHYL FORMAMIDE/CN
          E DIMETHYL FORMAMIDE/CN
          E T-BUTYL CYANOACETATE/CN
```

FILE 'HCAPLUS' ENTERED AT 01:44:10 ON 27 OCT 2004

=> s 13

```
L6      11 L3
```

=> s 13/prep

h eb c g cg b cg

eb

```

11 L3
3214460 PREP/RL
L7      11 L3/PREP
        (L3 (L) PREP/RL)

```

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.36	162.19

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 DICTIONARY FILE UPDATES: 25 OCT 2004 HIGHEST RN 769101-30-6

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> @ dimethylformamide/cn

E1	1	DIMETHYLFLUOROSILYL (TRICHLOROGERMYL) METHANE/CN
E2	1	DIMETHYLFORMALDEHYDE/CN
E3	1 -->	DIMETHYLFORMAMIDE/CN
E4	1	DIMETHYLFORMAMIDE 2,4-DINITROPHENYLHYDRAZONE/CN
E5	1	DIMETHYLFORMAMIDE AZINE/CN
E6	1	DIMETHYLFORMAMIDE COMPLEX WITH MOL. IODINE (1:1)/CN
E7	1	DIMETHYLFORMAMIDE COMPOUND WITH CARBON TETRACHLORIDE (1:1)/CN
		N
E8	1	DIMETHYLFORMAMIDE COMPOUND WITH SULFUR TRIOXIDE (1:1)/CN
E9	1	DIMETHYLFORMAMIDE COMPOUND WITH WATER (1:1)/CN
E10	1	DIMETHYLFORMAMIDE COMPOUND WITH WATER (2:1)/CN
E11	1	DIMETHYLFORMAMIDE CYCLIC ETHYLENE ACETAL/CN
E12	1	DIMETHYLFORMAMIDE DEMETHYLASE/CN

=> s @3

L8 1 DIMETHYLFORMAMIDE/CN

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	4.85	167.04

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FILE COVERS 1907 - 27 Oct 2004 VOL 141 ISS 18
FILE LAST UPDATED: 25 Oct 2004 (20041025/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l8/rct

27195 L8
2670391 RCT/RL

L9 4103 L8/RCT
(L8 (L) RCT/RL)

=> d his

(FILE 'HOME' ENTERED AT 01:37:40 ON 27 OCT 2004)

FILE 'REGISTRY' ENTERED AT 01:37:49 ON 27 OCT 2004

L1 STRUCTURE UPLOADED
L2 1 S L1
L3 5 S L1 FULL
L4 STRUCTURE UPLOADED
L5 18 S L4
E DIMETHYL FORMAMIDE/CN
E DIMETHYL FORMAMIDE/CN
E T-BUTYL CYANOACETATE/CN

FILE 'HCAPLUS' ENTERED AT 01:44:10 ON 27 OCT 2004

L6 11 S L3
L7 11 S L3/PREP

FILE 'REGISTRY' ENTERED AT 01:44:36 ON 27 OCT 2004

E DIMETHYLFORMAMIDE/CN
L8 1 S E3

FILE 'HCAPLUS' ENTERED AT 01:44:50 ON 27 OCT 2004

L9 4103 S L8/RCT

=> s l8 and l7

L10 1 L9 AND L7

=> d l10, ibib abs hitstr, 1

L10 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full	Chem
Text	References

ACCESSION NUMBER: 1999:794373 HCAPLUS
DOCUMENT NUMBER: 132:35620

TITLE: Preparation of substituted 3-cyanoquinolines as inhibitors of growth factor receptor protein tyrosine kinases (PTK)

INVENTOR(S): Wissner, Allan; Johnson, Bernard D.; Reich, Marvin F.; Floyd, Middleton B., Jr.; Kitchen, Douglas B.; Tsou, Hwei-ru

PATENT ASSIGNEE(S): American Cyanamid Co., USA

SOURCE: U.S., 80 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent

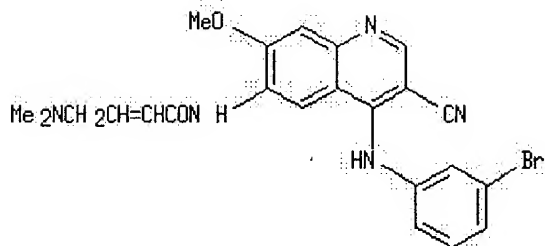
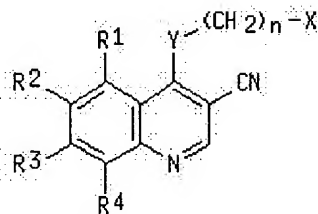
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6002008	A	19991214	US 1998-49718	19980327
PRIORITY APPLN. INFO.:			US 1997-41963P	P 19970403
OTHER SOURCE(S):	MARPAT 132:35620			

GI



AB This invention provides compds. having the formula (I; wherein: X is cycloalkyl which may be optionally substituted; or is a pyridinyl, pyrimidinyl, or Ph ring; wherein the pyridinyl, pyrimidinyl, or Ph ring may be optionally substituted; n is 0-1; Y is NH, O, S, or NR; R is alkyl of 1-6 carbon atoms; R1, R2, R3, and R4 are each, independently, hydrogen, halogen, alkyl, alkenyl, alkynyl, alkenyloxy, alkynoyloxy, hydroxymethyl, halomethyl, alkanoyloxy, alkenoyloxy, alkynoyloxy, alkanoyloxymethyl, alkenoyloxymethyl, alkynoyloxymethyl, alkoxymethyl, alkoxy, alkylthio, alkylsulphanyl, alkylsulfonyl, alkylsulfonamido, alkenylsulfonamido, alkynylsulfonamido, hydroxy, trifluoromethyl, cyano, nitro, carboxy, carboalkoxy, carboalkyl, phenoxy, Ph, thiophenoxy, benzyl, amino, hydroxyamino, alkoxyamino, alkylamino, dialkylamino, aminoalkyl, N-alkylaminoalkyl, N,N-dialkylaminoalkyl, phenylamino, benzylamino, etc.; R5 is alkyl which may be optionally substituted, or Ph which may be optionally substituted; R6 is hydrogen, alkyl, or alkenyl; R7 is chloro or bromo; R8 is hydrogen, alkyl, aminoalkyl, N-alkylaminoalkyl, N,N-dialkylaminoalkyl, N-cycloalkylaminoalkyl, N-cycloalkyl-N-

alkylaminoalkyl, N,N-dicycloalkylaminoalkyl, morpholino-N-alkyl, piperidino-N-alkyl, N-alkyl-piperidino-N-alkyl, azacycloalkyl-N-alkyl, hydroxyalkyl, alkoxyalkyl, carboxy, carboalkoxy, Ph, carboalkyl, chloro, fluoro, or bromo; Z is amino, hydroxy, alkoxy, alkylamino, dialkylamino). The compds. of the present invention inhibit the action of certain growth factor receptor protein tyrosine kinases (PTK) thereby inhibiting the abnormal growth of certain cell types. They are therefore useful for the treatment of certain diseases that are the result of deregulation of these PTKs, in particular as anti-cancer agents for the treatment of cancers expressing epidermal growth factor receptor (EGFR), mitogen activated protein kinase (MAPK), epithelial kinase (ECK), and kinase insert domain contg. receptor (KDR) in mammals and for the treatment of polycystic kidney disease in mammals. Thus, To a mixt. of 1.9 g (5.1 mmol) of 4-[(3-bromophenyl)amino]-7-methoxy-6-amino-3-quinolinecarbonitrile and 5.3 mL (31 mmol) of Hunig's base in 110 mL of dry THF at 0° C., with stirring, was added a THF soln. contg. 5.7 g (31 mmol) of 4-bromocrotonyl chloride dropwise. The mixt. was stirred for addnl. 0.5 h. After addn. 100 mL of satd. sodium chloride soln. was added to the reaction mixt., then it was extd. with Et acetate. The Et acetate soln. was dried over sodium sulfate and then was added to 40 mL of di-Me amine soln. (2.0 M in THF) at 0° dropwise and stirred an addnl. 0.5 h to give 4-Dimethylamino-but-2-enoic acid [4-(3-bromo-phenylamino)-3-cyano-7-methoxy-quinolin-6-yl]amide (II). II showed IC50 of 0.000008 µM against epidermal growth factor receptor kinase.

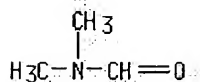
IT 68-12-2, DMF, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of substituted 3-cyanoquinolines as inhibitors of growth factor receptor protein tyrosine kinases (PTK) for treatment of cancers and polycystic kidney disease)

RN 68-12-2 HCAPLUS

CN Formamide, N,N-dimethyl- (8CI, 9CI) (CA INDEX NAME)



IT 27333-44-4P 214476-08-1P

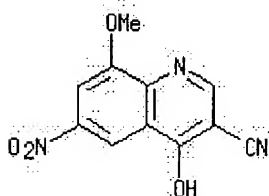
RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(prepn. of substituted 3-cyanoquinolines as inhibitors of growth factor receptor protein tyrosine kinases (PTK) for treatment of cancers and polycystic kidney disease)

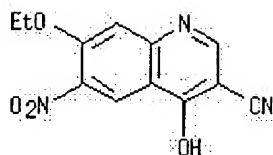
RN 27333-44-4 HCAPLUS

CN 3-Quinolinecarbonitrile, 4-hydroxy-8-methoxy-6-nitro- (8CI, 9CI) (CA INDEX NAME)



RN 214476-08-1 HCAPLUS

CN 3-Quinolinecarbonitrile, 7-ethoxy-4-hydroxy-6-nitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 01:37:40 ON 27 OCT 2004)

FILE 'REGISTRY' ENTERED AT 01:37:49 ON 27 OCT 2004

L1 STRUCTURE UPLOADED
 L2 1 S L1
 L3 5 S L1 FULL
 L4 STRUCTURE UPLOADED
 L5 18 S L4
 E DIMETHYL FORMAMIDE/CN
 E DIMETHYL FORMAMIDE/CN
 E T-BUTYL CYANOACETATE/CN

FILE 'HCAPLUS' ENTERED AT 01:44:10 ON 27 OCT 2004

L6 11 S L3
 L7 11 S L3/PREP

FILE 'REGISTRY' ENTERED AT 01:44:36 ON 27 OCT 2004

E DIMETHYLFORMAMIDE/CN
 L8 1 S E3

FILE 'HCAPLUS' ENTERED AT 01:44:50 ON 27 OCT 2004

L9 4103 S L8/RCT
 L10 1 S L9 AND L7

=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	7.12	174.16
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.70	-0.70

FILE 'CAOLD' ENTERED AT 01:45:24 ON 27 OCT 2004

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "[HELP USAGETERMS](#)" FOR DETAILS.

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

(FILE 'HOME' ENTERED AT 01:37:40 ON 27 OCT 2004)

FILE 'REGISTRY' ENTERED AT 01:37:49 ON 27 OCT 2004

```
L1      STRUCTURE UPLOADED
L2      1 S L1
L3      5 S L1 FULL
L4      STRUCTURE UPLOADED
L5      18 S L4
        E DIMETHYL FORMAMIDE/CN
        E DIMETHYL FORMAMIDE/CN
        E T-BUTYL CYANOACETATE/CN
```

FILE 'HCAPLUS' ENTERED AT 01:44:10 ON 27 OCT 2004

```
L6      11 S L3
L7      11 S L3/PREP
```

FILE 'REGISTRY' ENTERED AT 01:44:36 ON 27 OCT 2004

```
        E DIMETHYLFORMAMIDE/CN
L8      1 S E3
```

FILE 'HCAPLUS' ENTERED AT 01:44:50 ON 27 OCT 2004

```
L9      4103 S L8/RCT
L10     1 S L9 AND L7
```

FILE 'CAOLD' ENTERED AT 01:45:24 ON 27 OCT 2004

=> s l3 and l8

```
        0 L3
        17 L8
L11     0 L3 AND L8
```

=> file casreact

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.42	174.58
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-0.70

FILE 'CASREACT' ENTERED AT 01:45:42 ON 27 OCT 2004

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FILE CONTENT:1840 - 24 Oct 2004 VOL 141 ISS 17

```
*****
*
*   CASREACT now has more than 8 million reactions
*
```


*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

L12 STRUCTURE UPLOADED

=> d 112

L12 HAS NO ANSWERS

L12 STR

12
O M1

C 08

C 09

Page 1-A

PRO

C≡N
011 34

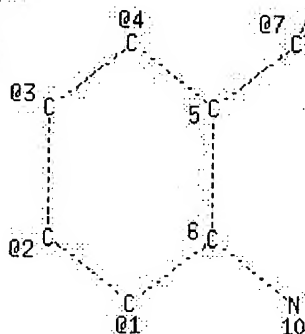
Page 1-B

40 41
39 C M3 C—C
M2 E3

Page 1-D

PRO

PRO
36
O
N 013
O
35



h eb c g cg b cg

eb

Page 1-F



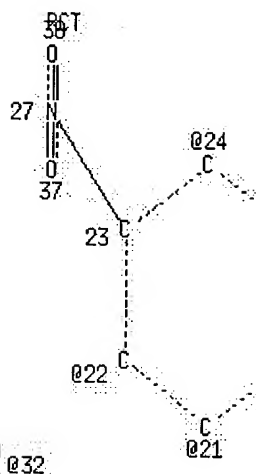
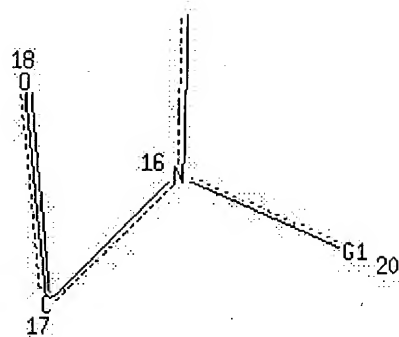
RRT



Page 2-E

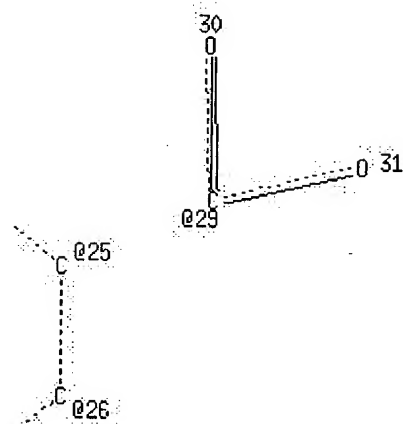
RCT

Page 2-F



RCT
Ak 33

Page 3-E



RCT
O28 N M2

Page 3-F

VAR G1=39/40

h eb c g cg b cg

eb

VPA 11-7/8/9 S
 VPA 13-2/3/4 S
 VPA 15-1/2/3 S
 VPA 28-21/25/26 S
 VPA 29-24/25/26 S
 VPA 32-21/22/24 S

NODE ATTRIBUTES:

HCOUNT	IS M1	AT	12
HCOUNT	IS M2	AT	28
HCOUNT	IS M3	AT	39
HCOUNT	IS M2	AT	40
HCOUNT	IS E3	AT	41
NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS R	AT	7
NSPEC	IS R	AT	8
NSPEC	IS R	AT	9
NSPEC	IS R	AT	10
NSPEC	IS C	AT	11
NSPEC	IS C	AT	12
NSPEC	IS C	AT	13
NSPEC	IS C	AT	14
NSPEC	IS C	AT	15
NSPEC	IS C	AT	16
NSPEC	IS C	AT	17
NSPEC	IS C	AT	18
NSPEC	IS C	AT	19
NSPEC	IS C	AT	20
NSPEC	IS R	AT	21
NSPEC	IS R	AT	22
NSPEC	IS R	AT	23
NSPEC	IS R	AT	24
NSPEC	IS R	AT	25
NSPEC	IS R	AT	26
NSPEC	IS C	AT	27
NSPEC	IS C	AT	28
NSPEC	IS C	AT	29
NSPEC	IS C	AT	30
NSPEC	IS C	AT	31
NSPEC	IS C	AT	32
NSPEC	IS C	AT	33
NSPEC	IS C	AT	34
NSPEC	IS C	AT	35
NSPEC	IS C	AT	36
NSPEC	IS C	AT	37
NSPEC	IS C	AT	38

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 11 12 13 14 15 16 17 18 27 28 29 30 31 32 33 34 35
 36 37 38 39 40 41

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 41

STEREO ATTRIBUTES: NONE

=> s 112

SAMPLE SEARCH INITIATED 01:51:30 FILE 'CASREACT'

SCREENING COMPLETE - 0 REACTIONS TO VERIFY FROM 0 DOCUMENTS

100.0% DONE 0 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 0 TO 0

PROJECTED ANSWERS: 0 TO 0

L13 0 SEA SSS SAM L12 (0 REACTIONS)

=> s 112 full

THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 102.30 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 01:51:36 FILE 'CASREACT'

SCREENING COMPLETE - 4 REACTIONS TO VERIFY FROM 1 DOCUMENTS

100.0% DONE 4 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

L14 0 SEA SSS FUL L12 (0 REACTIONS)

=>

L15 STRUCTURE UPLOADED

=> d 115

L15 HAS NO ANSWERS

L15 STR

0 M1

C 08

C 09

Page 1-A

C=N

@11 34

Page 1-B

40

39 C M3 C

M2

E3

Page 1-D

h

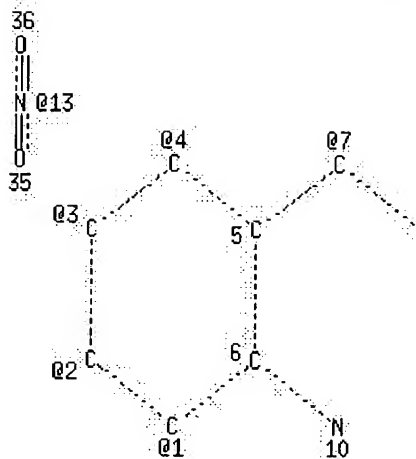
eb c

g cg b

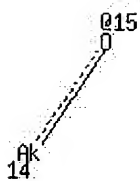
cg

eb

012

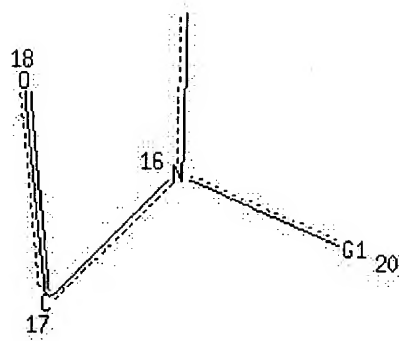


Page 1-F

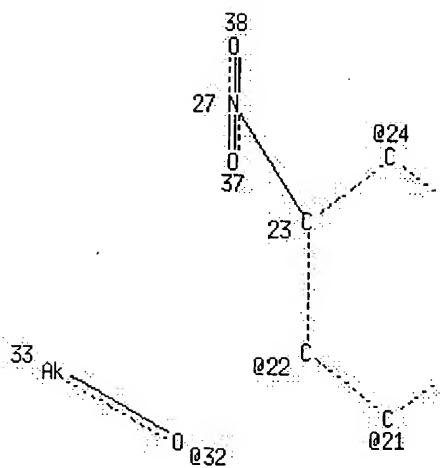


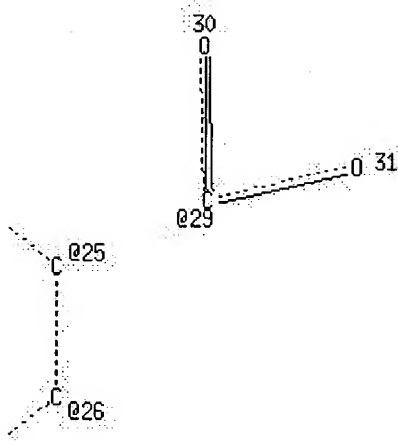
19
G1

Page 2-E



Page 3-E





028 N M2

Page 3-F

VAR G1=39/40

VPA 11-7/8/9 S

VPA 13-2/3/4 S

VPA 15-1/2/3 S

VPA 28-21/25/26 S

VPA 29-24/25/26 S

VPA 32-21/22/24 S

VPA 12-7/8 S

NODE ATTRIBUTES:

HCOUNT	IS M1	AT	12
HCOUNT	IS M2	AT	28
HCOUNT	IS M3	AT	39
HCOUNT	IS M2	AT	40
HCOUNT	IS E3	AT	41
NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS R	AT	7
NSPEC	IS R	AT	8
NSPEC	IS R	AT	9
NSPEC	IS R	AT	10
NSPEC	IS C	AT	11
NSPEC	IS C	AT	12
NSPEC	IS C	AT	13
NSPEC	IS C	AT	14
NSPEC	IS C	AT	15
NSPEC	IS C	AT	16
NSPEC	IS C	AT	17
NSPEC	IS C	AT	18
NSPEC	IS C	AT	19
NSPEC	IS C	AT	20
NSPEC	IS R	AT	21
NSPEC	IS R	AT	22
NSPEC	IS R	AT	23
NSPEC	IS R	AT	24
NSPEC	IS R	AT	25
NSPEC	IS R	AT	26
NSPEC	IS C	AT	27
NSPEC	IS C	AT	28

NSPEC IS C AT 29
 NSPEC IS C AT 30
 NSPEC IS C AT 31
 NSPEC IS C AT 32
 NSPEC IS C AT 33
 NSPEC IS C AT 34
 NSPEC IS C AT 35
 NSPEC IS C AT 36
 NSPEC IS C AT 37
 NSPEC IS C AT 38
 DEFAULT MLEVEL IS ATOM
 MLEVEL IS CLASS AT 11 12 13 14 15 16 17 18 27 28 29 30 31 32 33 34 35
 36 37 38 39 40 41
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RSPEC I
 NUMBER OF NODES IS 41

STEREO ATTRIBUTES: NONE

=> s l15

SAMPLE SEARCH INITIATED 01:52:41 FILE 'CASREACT'
 SCREENING COMPLETE - 1 REACTIONS TO VERIFY FROM 1 DOCUMENTS

100.0% DONE 1 VERIFIED 0 HIT RXNS 0 DOCS
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED VERIFICATIONS: 1 TO 79
 PROJECTED ANSWERS: 0 TO 0

L16 0 SEA SSS SAM L15 (0 REACTIONS)

=> s l15 full

THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 102.30 U.S. DOLLARS
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
 FULL SEARCH INITIATED 01:52:46 FILE 'CASREACT'
 SCREENING COMPLETE - 50 REACTIONS TO VERIFY FROM 12 DOCUMENTS

100.0% DONE 50 VERIFIED 0 HIT RXNS 0 DOCS
 SEARCH TIME: 00.00.01

L17 0 SEA SSS FUL L15 (0 REACTIONS)

=>